Glutaric acid, phenethyl undecyl ester

Inchi: InChI=1S/C24H38O4/c1-2-3-4-5-6-7-8-9-13-20-27-23(25)17-14-18-24(26)28-21-19-22-15
InchiKey: MCOVFNUYGSDRNK-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-204.23	kJ/mol	Joback Method
hf	-791.76	kJ/mol	Joback Method
hfus	57.53	kJ/mol	Joback Method
hvap	89.61	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.017		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1041.25	kPa	Joback Method
rinpol	2950.00		NIST Webbook
tb	927.78	K	Joback Method
tc	1136.42	K	Joback Method
tf	530.98	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.96	J/mol×K	927.78	Joback Method
cpg	1192.57	J/mol×K	1101.65	Joback Method
cpg	1180.56	J/mol×K	1066.87	Joback Method
cpg	1167.34	J/mol×K	1032.10	Joback Method
cpg	1152.87	J/mol×K	997.33	Joback Method
cpg	1137.09	J/mol×K	962.55	Joback Method
cpg	1203.40	J/mol×K	1136.42	Joback Method
dvisc	0.0000302	Pa×s	927.78	Joback Method
dvisc	0.0000398	Pa×s	861.65	Joback Method

dvisc	0.0000549	Pa×s	795.51	Joback Method
dvisc	0.0000804	Pa×s	729.38	Joback Method
dvisc	0.0001269	Pa×s	663.25	Joback Method
dvisc	0.0002217	Pa×s	597.11	Joback Method
dvisc	0.0004449	Pa×s	530.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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